

**Abstract of the Disclosure**

Polypeptides containing the PIN1 peptidyl-prolyl isomerase domain but not containing the PIN1 WW domain are described. Also described are crystal structures 5 of these polypeptides, including the crystal structure of a PIN1 PPIase:ligand complex. The structure coordinate data derived from these crystals provides a three-dimensional description of the substrate-binding site of PIN1 peptidyl-prolyl isomerase useful in drug discovery and design for the identification and design of modulators of PIN1 peptidyl-prolyl isomerase activity.